

Development of Advanced Numerical Algorithms and Physical Parameterizations Within the Regional Ocean Modeling System (ROMS)

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LONG-TERM GOALS

The primary goals of this research project are to systematically assess the performance and refine the numerical algorithms, physical parameterizations, and computational strategies used in Regional Ocean Modeling System (ROMS). ROMS is a relatively new oceanic model, with parallel and loosely-coordinated developments between Dr. Hernan Arango (Rutgers) and us. It has established itself as a viable community model with a growing number of research users.

OBJECTIVES

The objectives of this project are the following: (1) consolidation of the computational kernel of ROMS with respect to pressure-gradient force, equation of state, embedded grids, time-stepping, vertical-mode coupling, and biological modeling; (2) further development of parallelization capabilities, including a hybrid combination of message-passing and shared memory methods, plus migration of ROMS to the IBM SP computer and implementation of generalized (unstructured) message-passing; (3) application of polynomial reconstruction schemes to advection, dissipation, and mixing algorithms; (4) improvements of the K-Profile Parameterization (KPP) for surface and bottom boundary layer mixing; and (5) development of a dynamically adaptive vertical grid as a generalization of the present sigma-coordinate grid, to combine the distinctive advantages of height, density, and terrain-following coordinates.

APPROACH

The primary design goal for ROMS is to produce limited-area, high-resolution, realistic coastal simulations in an efficient manner on parallel computers. The technical approach is computational simulation of oceanic fields for velocity, temperature, and salinity; chemical concentrations of nutrients, O₂, CO₂, etc.; planktonic populations; and mobile sediments. ROMS is based on the hydrostatic Primitive Equations in terrain-following curvilinear coordinates with a free upper surface. It contains a variety of innovative algorithms, including an advection operator designed to reduce dispersive errors and, consequently, excessive dissipation rates, thereby effectively boosting the resolution on a given grid (Shchepetkin & McWilliams, 1998). The boundary-value problems that are our focus are for various regional domains along the North American West Coast (*e.g.*, Marchesiello *et al.*, 2002) with specified

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surface forcing fields and boundary data, including the output from a whole-Pacific ROMS configuration. The boundary data are imposed by adaptive open boundary conditions (Marchesiello *et al.*, 2001). We have developed and implemented a hierarchical embedding capability for the local, fine-resolution grid in a sub-domain within the coarse-resolution grid spanning the entire domain (Penven *et al.*, 2002). Key researchers at UCLA on this project are Meinte Blaas, Xavier Capet, Patrick Marchesiello, James McWilliams, Pierrick Penven, and Alexander Shchepetkin, as well as Nicholas Gruber, Hartmut Frenzel, and Keith Stolzenbach for biogeochemical and sedimentary issues.

WORK COMPLETED

During the past year we have made good progress on objectives (1), (2), and (4)—see Results below. For objective (3) we expect to write a paper soon on lateral mixing in general curvilinear coordinates. Work on objective (5) is deferred.

RESULTS

Sigma-coordinate pressure gradient problem: We completed this development, including a new treatment of the seawater Equation of State (EOS), test problems under realistic simulation conditions, and a proof of discrete energetic consistency to the case of higher than second-order accuracy. In our new treatment of the compressibility effect in the seawater EOS, we abandon computation of *in situ* density in favor of density gradients formulated in terms of adiabatic differences, which allows us to bring the mathematical criterion of grid-scale smoothness of the discrete field (needed to avoid spurious oscillations of polynomial interpolants) into the context of positive-definiteness of density stratification. This work is now completed (Shchepetkin & McWilliams, 2002a). An accompanying intercomparison

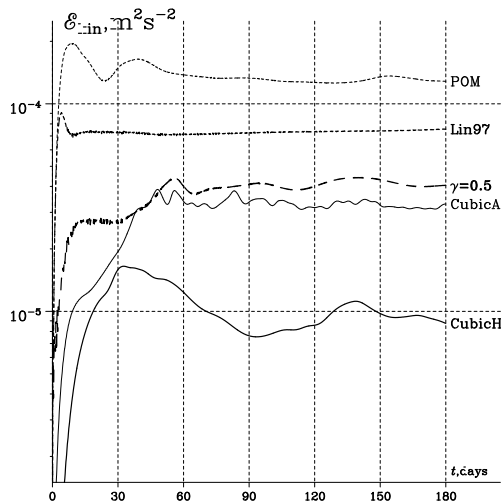


Figure 1: Volume-averaged kinetic energy of spurious flow generated by pressure-gradient error in a flat-stratification seamount test problem as function of time (in days) for five different pressure-gradient schemes. *POM*—density-Jacobian from Princeton Ocean Model; *Lin 97*—finite-volume method of Lin (1997); $\gamma=0.5$ —weighted Jacobian of Song (1998) with weighting coefficient decreased by a factor of 2 (*i.e.*, half-and-half average of *POM* and Song (1998) Jacobians, which is the optimal weighting in terms of error among all possible linear combinations of these Jacobians; *Cubic A*—a fourth-order accurate density Jacobian scheme using algebraic averaging of elementary differences to estimate density derivatives at density points; *Cubic H*—same as *Cubic A*, but with harmonic averaging to constrain monotonicity of cubic polynomial interpolants for density field.

for a wider range of discretization methods has also been published, Ezer *et al.*, (2002).

Time-stepping and time-splitting algorithms: At present the UCLA ROMS model employs a predictor-corrector time-step for both barotropic and baroclinic modes, with forward-backward feedback between the free-surface/tracer and momentum equation at every stage to increase the stability limits in the time-step size associated with internal waves. A forward step is used for lateral viscosity and diffusion and a backward step for vertical diffusion. In both cases viscous/diffusive terms are computed

only once per time step to save the computational costs of the rotation of horizontal mixing terms (necessary due to sigma coordinates) and the vertical mixing parameterization. A new version of the barotropic mode using a generalized forward-backward time step is now available and has been shown to be more efficient than predictor-corrector in terms of stability limit vs. computational cost. Also, the barotropic-baroclinic mode coupling can now occur during either predictor or corrector stages of the baroclinic time step (both versions are available). The predictor-coupled mode algorithm uses forward-in-time extrapolation of the mode-coupling terms (vertically integrated r.h.s. of 3D momentum equations minus r.h.s. computed from barotropic variables), in a manner similar to an Adams-Bashforth time step, before the coupling terms are applied as forcing at every step of barotropic mode. No such extrapolation is required for the corrector-coupled version, because, after the predictor stage is complete, the newly computed 3D variables are already time-centered half-way between the n and $n + 1$ time levels. This also makes it possible to retain only terms critical for the computational stability of internal waves and advection during the predictor stage for the 3D momentum equations. This mitigates computational cost. This analysis is nearly finalized, and an associated manuscript is being prepared (Shchepetkin & McWilliams, 2002b).

Parallel code design and portability issues: As stated in the proposal, UCLA ROMS is committed to supporting both shared-memory and MPI implementations within the same source code. However, for performance reasons our implementation of the shared-memory capability was bound to the SGI Origin 2000 that historically has been our primary production environment. After the release of Open MP 2.0 Fortran Specification standard, <http://www.openmp.org>, and the subsequent appearance of compilers supporting the new standard, it became possible to create a portable code without compromising its performance. Correspondingly, our shared-memory implementation of ROMS was redesigned to comply with Open MP 2.0 standard. This direction of work is in mature stage at this moment, with our embedded-gridding capability now being converted. Besides the SGI Origin 2000, the new shared-memory implementation was tested and proven to work "out-of-box" on platforms like IBM and Intel. The last opportunity is especially intriguing due to recent rapid progress on low-cost, commodity hardware, which in fact may outperform high-end supercomputers in terms of processing power per CPU, provided that codes are properly optimized to take into account cache effects, Fig. 2. The use of commodity PC hardware is often associated with Linux clusters running MPI-parallelized codes that mostly conform to one subdomain – one processor strategy. Fig. 2 shows in addition that one may take advantage of multiple subdomains per processor option of ROMS and significantly (by a factor of 2.5) improve the utilization of hardware.

Transition to Fortran 90: This effort is primarily motivated by our embedded-gridding project (where the use of Fortran 90 features is indispensable) and is closely related to the prototype code development, as well as reflecting recent trends in compiler technology. It is also our desire to keep the embedded and non-embedded codes as close as possible so that implementation of algorithms can be quickly transferred from one to the other. Decision making associated with this change is rather complex since in present F90 compilers many features actually impede computational performance. Therefore, we assume a balanced approach that allows a smooth transition to F90 whenever it is advantageous (*e.g.*, an irreversible transition to F90-only environment would impede the use of ROMS on Linux computers, thus cutting off a relatively wide and growing portion of user community). During the last year we developed a series of automatic tools to identify and convert types of variables and constants (automatic promotion to double precision, if so desired), to convert F77 common blocks to F90 modules, etc. These

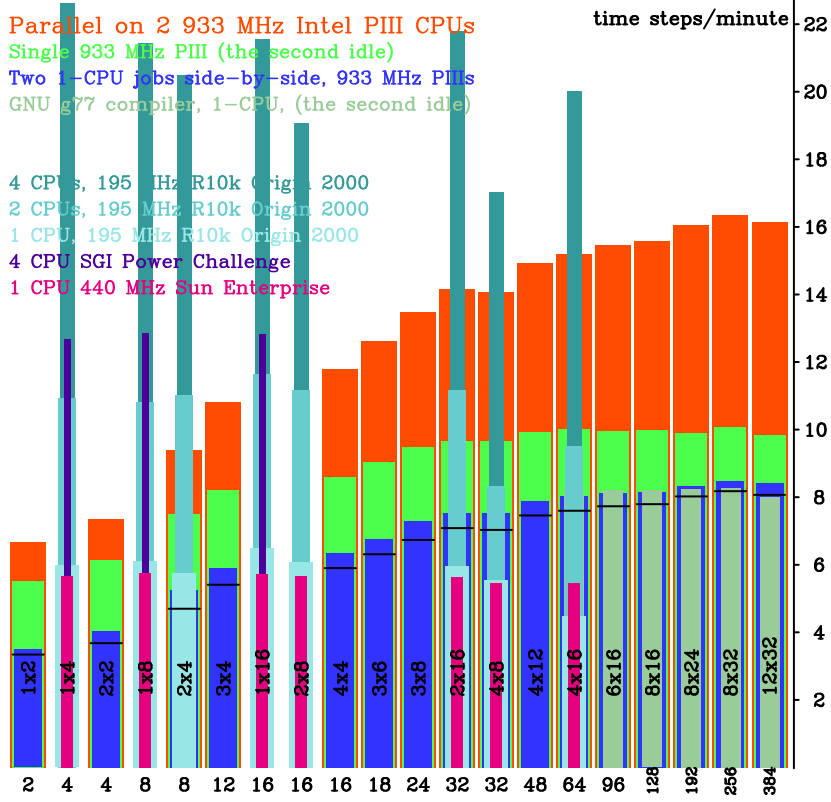


Figure 2: Computational performance of ROMS code as a function of subdomain partitioning (blocking) policy on different hardware platforms for 3/4 degree Atlantic Ocean test configuration. Grid resolution is $128 \times 128 \times 20$, resulting in a 100 MB memory storage. Horizontal axis—number of subdomains (two-dimensional arrangement is written in each column in $N_X \times N_Y$ format); vertical axis—computational speed expressed in model time steps per minute of wall clock time. In all cases parallelization is done via OpenMP and no adjustments to the code are made other than choosing different number of subdomains. Intel 933 MHz is a dual-processor Pentium III SMP machine running Linux and using Intel IFC 6.0 FORTRAN 90/95 compiler. Strong dependency of computation performance from number of subdomains for Intel platform is explained by cache effects due to combination of small cache, fast processors and limitation by memory bandwidth, which is by far the dominant factor for optimization strategy in this case. For all other platforms the effect is less significant, and, in fact the most significant influence on performance can be traced to the side effects due to shortening of innermost loops when decreasing subdomain size. Nevertheless, for a properly optimized code (number of subdomains is chosen to make subdomains sufficiently small to fit into cache), even the previous generation of Intel platforms tends to outperform the other computers presented here in terms of processing power per CPU, despite the fact that its cost is only a small fraction of the cost of others. We have preliminary experience with newer 2 GHz P4 CPU, which makes this comparison is even more striking (P4 SMPs are just emerging on the market but not yet widely available).

tools may be used both as code-development instruments to make permanent changes, as well as at compile time to make reversible automatic changes in order to ensure the portability of the code.

KPP of vertical mixing: Relative to the original publication (Large, *et al.*, 1994) and subsequent

implementation in NCAR's and other z -coordinate general circulation models, the KPP vertical mixing parameterization was modified in several aspects in order to make it suitable for the framework of terrain-following coordinate of ROMS. This is due to B-C grid difference and, more importantly, due to the discretization algorithms of a sigma-grid with their horizontally variable vertical resolution and concerns about hydrostatic consistency, which, unlike z -coordinate models, do not allow an arbitrary increase of vertical resolution. Consequently, the KPP scheme has to cope with a coarser vertical resolution, resulting in tougher requirements on the vertical discretization methods. Thus, instead of estimating Richardson number via finite differences at every grid point and then interpolating it linearly to determine the boundary layer depth (where a bulk Richardson number crosses its critical value), the problem is reformulated in terms of low-order polynomial fits of prognostic variables—velocity and density—which tend to possess a smoother behavior than Richardson number, resulting in more accurate positioning of boundary layer edge. This procedure alone significantly mitigates the "stepiness" in boundary layer deepening, as well as eliminates any necessity of spatial smoothing of Richardson number for numerical reasons (a common practice in z -coordinate models). We are now doing a general reconsideration of the physical rules in KPP, specifically focusing on how high-frequency surface forcing systematically increases the boundary layer depth when the stratification is strong.

IMPACT/APPLICATIONS

The validated technical innovations in our evolving model are prototypes for future improvements in operational observing-system, data-assimilation, and prediction capabilities. The scientific understanding of the coastal oceans is relevant to the U.S. Navy's missions.

TRANSITIONS

One tangible measure of the utility of our results is that other researchers are either using our evolving ROMS code or adapting its algorithms for their own code. Current users of our version of ROMS include Chao and Li (NASA/JPL), Miller and Cornuelle (SIO), Moisan (NASA/Wallops), and the Monterey Bay NOPP SCOPE team—Chavez (MBARI), Chai (Maine), *et al.*, Arango and Haidvogel (Rutgers) have adapted many features for their version of ROMS. In the near future we anticipate additional users, partly through the ONR-sponsored, terrain-coordinate model development project (TOMS). We are contributing useful knowledge about coastal modeling methodology and phenomena through published papers.

RELATED PROJECTS

Our recent venture into coastal oceanography now extends into several related projects. We began with a focus on the Southern California Bight, especially with regard to its water quality [a California Sea Grant project]. We are just completing a ONR project on developing the embedded gridding capability for ROMS. We have a joint project with Chao [NASA/JPL] on using embedded grids in ROMS for studying Eastern and Western Boundary Current interactions with the North Pacific gyres [NASA]. We have a project jointly with Moisan (NASA), Miller and Cornuelle (SIO), and Haidvogel and Wilkin (Rutgers) to model the coastal carbon cycle [NASA]. We are partners in the NOPP SCOPE project for developing models and analyses for the Monterey National Marine Sanctuary. We have also submitted a proposal to ONR to participate in the Autonomous Ocean Sampling Network II field experiment in summer, 2003.

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